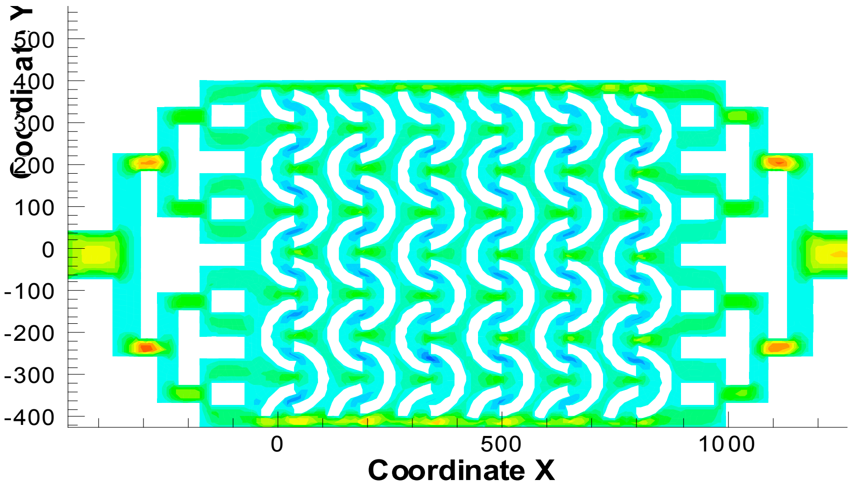
Louisiana EPSCoR BioTransport Processes

Development of computational and visualization techniques for microfluidics device design, MD and CFD theory and simulations, fluid transport in vessels and tissue, and flow/structure interactions.

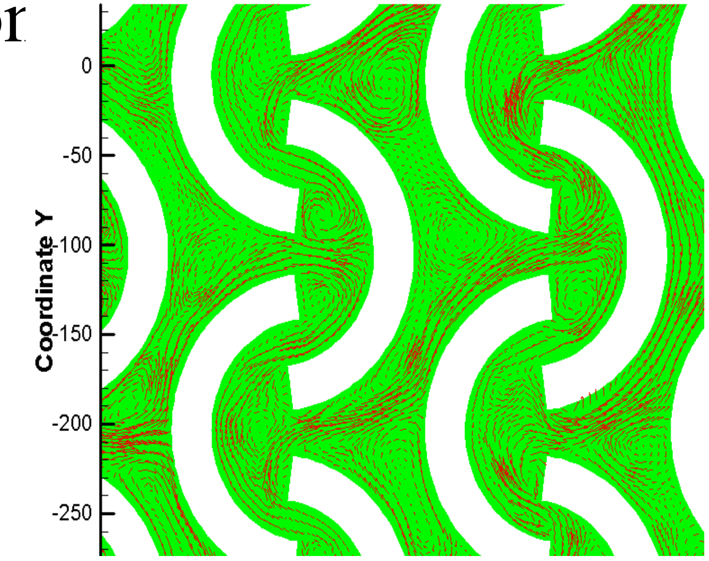
Bio-Sensor transport processes

Leaders:
Computation: Cortez, Gaver, Bishop (Tulane)
Experiments: Blake (Tulane), Soper (LSU)

Computational studies of materials critical for nanoscale interactions; optimal microfluidics device design, molecular dynamics interaction



a.



b.

Micromanufacturing at IfM

Leader: Varahramyan (LaTech)

- **Nanoassembly Techniques:** Layer-by-Layer Assembly, Molecular Recognition-Based Self-Assembly, Self-Assembled Monolayers (SAM), Nanoassembly by Step-Wise Polymerization
- **Nanopatterning Techniques:** X-ray Lithography, E-beam Lithography, Nanoimprint Lithography, Molecular Imprinting
- **Electroless Deposition Techniques** with Charged Nanoparticles
- **Measurement and Characterization Tools**
- **Microfluidic devices**

Convection/Diffusion and Mixing

Simulations will be conducted based upon Stokes Flow approximations using the boundary element method, immersed boundary method and method of regularized Stokeslets (as appropriate).

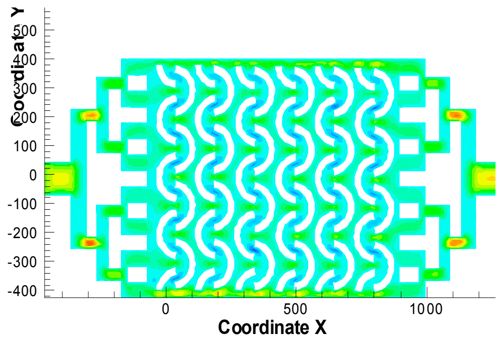
- **Toolkits** for data, computation needed for LONI environment - <u>links directly to biological experiments</u>.
- **Collaboration** with CAMD, LA Tech IfM, medical centers

$$\frac{\partial \varphi}{\partial t} + \vec{u} \cdot \nabla \varphi = D \Delta \varphi + R$$

$$\nabla P = \mu \nabla^2 \vec{u}, \quad \nabla \bullet \vec{u} = 0$$

$$R_{as} = K_s^b \varphi_s \varphi_a - K_s^r \varphi_{as}$$

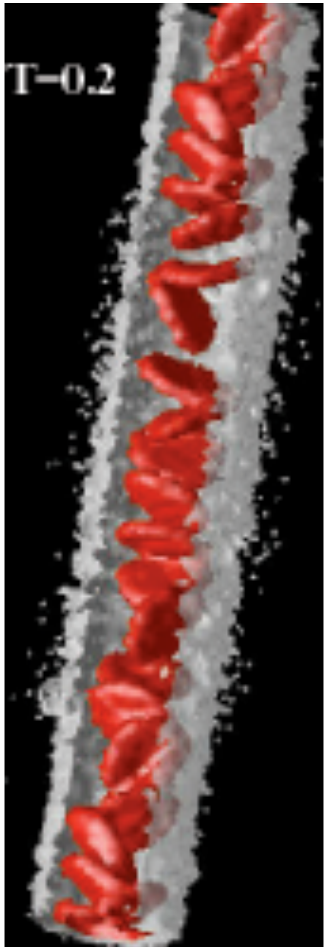
$$R_s = K_s^r \varphi_{as} - K_s^b \varphi_s \varphi_a$$



Bio-Transport Processes: Multi-Scale Simulations

Leader: Acharya (LSU)

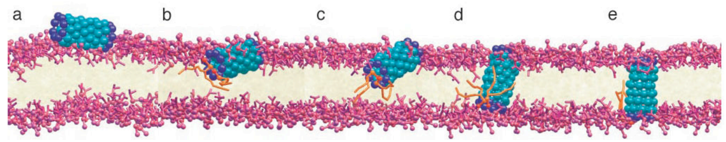
- Project Goals
  - Models for transport of oxygen and flow in blood vessels
- Scientific/Technology Challenges
  - Complex geometries with accommodation
  - Multi-scale simulation
  - Tera-scale and potential peta-scale computations
- Technical Approach
  - Continuum models in major blood vessels transport
  - Consumption across vessel walls, vessel accommodation
  - Boltzmann simulations in capillaries (non-continuum)
  - Mesoscopic simulations for property evaluation (coarse-graining)
  - Coupled atomistic-continuum hybrid model



Control of Transport through Biological Membranes using Nanoparticles (NP)

Leaders: Bishop (Tulane), Moldovan (LSU)

M. Klein et al., Proc of the Nat. Acad. of Sci. , 2004

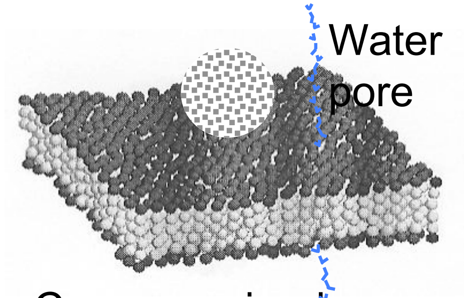


Relevance

• Understanding mechanisms of trans-membrane species delivery, gene therapy and membrane pore formation

Scientific Issues

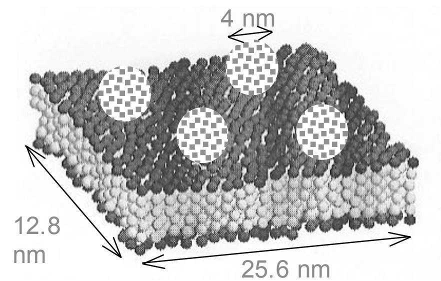
• NP-biomembrane Interaction
• Effect on hydration forces
• Water pore formation and stability



Coarse grained membrane model

Scientific/Computational Challenges

• Multi NP-biomembranes investigated with coarse graining
• Improve coarse grained computational models
• Develop new hybrid atomistic/coarse-grained/continuum models



Transport Processes Organization

Gaver/Cortez

(coordinators)

Convection/Diffusion Fluid-Structure

Tulane Team:
(Gaver/Cortez)

Multi-scale

LSU Team:
(Acharya)

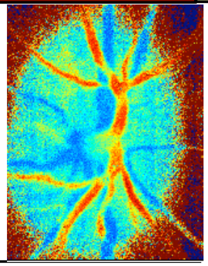
Micromanufacturing

LaTech Team:
(Varahramyan)

MD

Tulane: (Bishop Ashbaugh)
LSU: (Moldovan)
UNO: (Rick)

Bio-Transport Processes: Computational Challenges



- Complex accommodating grids (WP4)
  - Dynamic grid (ALE, IBM)
  - Flow-structure interaction (FEM, MPM, BEM)
- Multi-scale Simulation (WP4)
  - Continuum CFD (CFD Toolkit)
  - Molecular Dynamics (MD Toolkit)
  - Coarse-Graining/Mesoscale (Meso Toolkit)
  - Up-scaling/Information Transfer across Scales (Interfaces)
- Tera and peta-scale computing (WP1)
- Multi-scale visualization tools (WP3)

Deliverables: Bio-Transport

Overarching Goal: Improved understanding of the multi-scale physical mechanisms for flow and transport in biosensors and vessels/tissues

- **CFD continuum code** for bio-transport, tissue/wall-accommodation. This requires analysis of fluid-structure interaction, deforming grid structure, species and flow transport
- **Mesoscopic code** (Boltzman, coarse-grained MD) for relevant bio-transport applications (oxygen transport in capillary, species/particle transport across vessel/tissue walls) including non-continuum effects
- **Molecular Dynamics** (MD) code for transport across cell/lipid boundaries, antibody/analyte interactions
- **Interface algorithms:** Up-scaling/information transfer across scales
- **Integration** into *CyberTools* WorkPackages
- Tera- and peta-scale grand **challenge problems** in biotransport that take advantage of the computational hardware and middleware (WP'S)

Timeline: Bio-Transport/*CyberTool* Coordination

- **Year One:** Environmental scan of existing CFD tools and/or development of new CFD tools for the simulation of viscous flow and transport in irregular and compliant geometries, and MD simulations of small molecule interactions with biomembranes. The development and integration of toolkits for MD simulations and CFD simulations
- **Year Two:** Full CFD simulations across LONI of biosensor systems the oxygen transport in arterial vessels with available property data. MD simulations across LONI of small molecule and nano particle transport. Complete integration of CFD and MD toolkits (year two).
- **Year Three:** Toolkit driven CFD and MD simulations across LONI to further our understanding of multiscale bio-transport processes. Integrated CFD-MD simulations of bio-transport process.

Personnel: Bio-Transport/*CyberTool* Coordination

WP4:

- **Cactus-based Toolkits** (1 Allen postdoc, 1 Allen grad, 1 Jha grad, .5 Acharya postdoc, .5 Acharya grad, .5 Gaver grad, .5 Cortez grad)
  - **CFD Toolkit.** The CFD toolkit will be based on work started for the coastal modeling project. This will be expanded to support different fluid systems, structured and unstructured meshes, and application domains. In addition to the effort outlined **0.5 Allen postdoc, 1 Allen Grad, Tyagi, 0.5 Acharya posdoc, 0.5 Grad from Acharya and Tulane will be assigned to work on this project.** The toolkit will be developed in 3 releases
  - **MD Toolkit.** MD toolkit will be developed based on needs of the projects. First phase will be design and assessment of Charm++ or NAMD as a driver for Cactus. In addition to the effort outlines **0.5 Allen postdoc, CCT's Jha and 0.5 grad from Tulane** will work together to develop this toolkit in three releases.